

# Technology Opportunity

## Computer Simulation of Chemically Reacting Flows With Sprays

The computational fluid dynamics code ALLSPD-3D provides a numerical tool for simulating a wide variety of chemically reacting and nonreacting flows. Simulations provide detailed information on important quantities such as velocity, temperature, and concentrations of various chemical species within the flow domain of interest.

### Potential Commercial Uses

- Improve design of industrial furnaces, incinerators, gas turbine combustors
- Model flow in gas-phase chlorination reactors
- Support analysis of fire-suppression systems
- Simulate flow in fuel-injection systems and nozzles
- Investigate flow in microfluidic devices
- Analyze exhaust systems and determine emissions
- Model spray coating processes
- Assist in design of HVAC/climate control systems
- Study options for underhood engine cooling or brake cooling

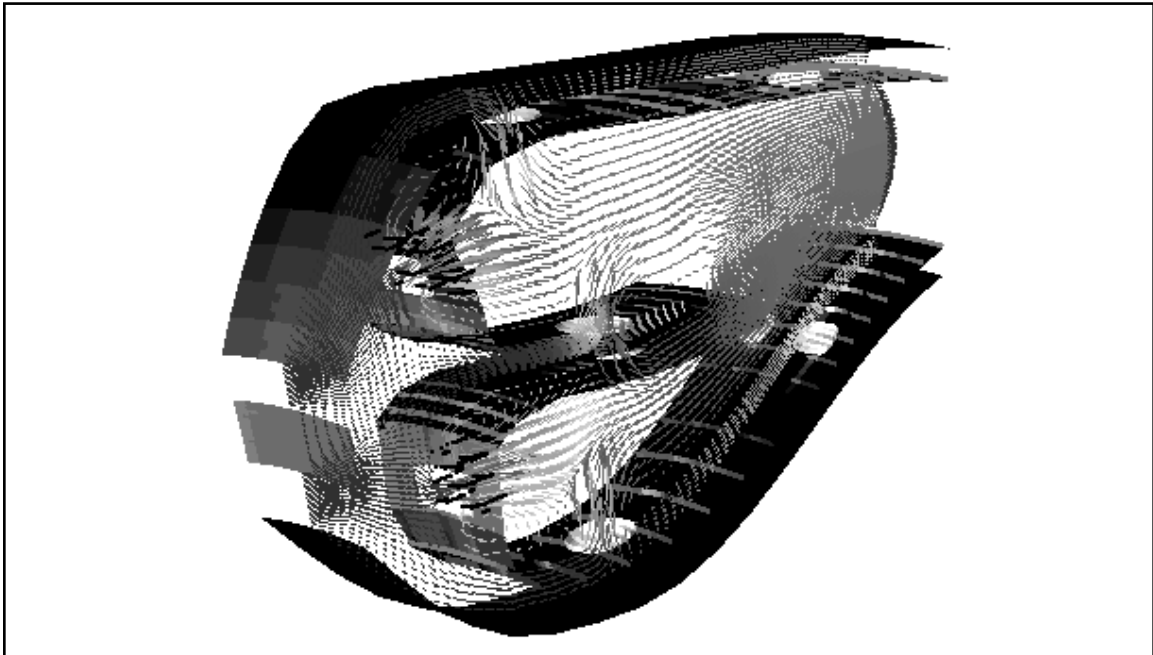


Figure 1.—Simulation of an aircraft-engine combustor flow showing velocity vectors shaded by temperature along a plane in the center of the combustor.



## Benefits

- Is low cost
- Reduces design-cycle time and cost with easily performed "what-if" or parametric studies
- Is supported on several UNIX platforms
- Provides graphical user interface for problem setup and postprocessing
- Permits complex geometry modeling
- Incorporates advanced physical models for turbulence, chemistry, sprays, radiation
- Simulates low-speed and high-speed flows

## The Technology

ALLSPD-3D is a computational fluid dynamics (CFD) code that was developed primarily for simulating chemically reacting flows with sprays in aircraft-engine combustors; however, it is applicable to a wide variety of reacting and nonreacting flows. The code is easily compiled to run in serial or parallel modes on several UNIX platforms. It is primarily written in FORTRAN, but much of the parallel coding is in C. The numerics of ALLSPD-3D are based on modern compressible algorithms to take advantage of advances made in CFD during the past two decades. ALLSPD-3D also includes a spray model to calculate the transport of liquid droplets within the gas-phase flow. ALLSPD-3D has been in development since 1991, with a two-dimensional version released in 1993 and a three-dimensional version released in 1995. A new version incorporating several upgrades is scheduled for release in 1997. Several validation test cases have been

performed, such as the simulation depicted in figure 1. Documentation, source code and sample input/output files are available in several formats, including cartridge tapes or anonymous ftp (file transfer protocol).

## Options for Commercialization

Release of the computational fluid dynamics code ALLSPD-3D is restricted to domestic organizations whose major computational activity is conducted within the United States. Low-cost technical support is provided by the ALLSPD team. Documentation and other information on the code are available to anyone, via the World Wide Web page at <http://www.lerc.nasa.gov/WWW/IFMD/allspd/>.

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## Key Words

Computational fluid dynamics  
Chemically reacting flows  
Sprays



National Aeronautics and  
Space Administration  
Lewis Research Center